Study of the Morse Fluid

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During recent years methods have been developed of molecular numeric simulation such as molecular Dynamics and Monte Carlo. Both are important tools in computational physics, basically the use of simulations has provided of results not presented by any theoretical development. It is known that for a potential like that of square- well, the phase diagram presents a region of transition gas-liquid with a metastable behavior. We chose the potential of Morse basically because is similar to Lennard Jones potential but the manipulation of their width is given as a function of a single parameter. The Morse potential has the advantage of being continuous and it has an exact solution for the Schroedinger's equation and is short range. Originally this potential was used in the study of diatomic molecules, however upon changing the value of their parameter the basic form of the potential alone modify in their width it is a reason that we used it alternating in comparison with the square-well potential.

Preliminary, we calculated the function of velocity autocorrelation using molecular dynamic for 500 and 864 particles in the microcanonical ensemble for different values of density and of the range. We found that the velocity autocorrelation function presents a similar behavior to those reported for potentials of long range That is an oscillatory behavior, but we must recall that the potential is a short range kind. Now we studied the phase diagram of the system and hoped that when the width of the potential diminishes the functions of correlation clerks of the time they are similar to that of hard sphere and that the correlation functions present effects on the rest of the particles.